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Title: MESOSCALE MODELLING OF SHOCK INITIATION IN HMX-BASED EXPLOSIVES

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Mesoscale Modelling of Shock Initiation in HMX-Based Explosives

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Outline

- Motivation

- Model:

    - Equations of state

    - Constitutive models

    - Reaction rates

- Calibration and performance:

    - PBX 9501 run distance

    - PBX 9404 run distance

    - EDC37 run distance

    - PBX 9404 velocity history

    - EDC37 metal driving

- Conclusions

Motivation: predictive capability

Want to predict initiation, detonics and performance given:

- Variations in composition

- Variations in morphology

- Different loading conditions

Previous work on PBX and ANFO: need physically-based model rather than just mechanical calibrations.

Overview of model

hydrocode cell

regions of diff

thermal
equilibration:
transfer internal
energy
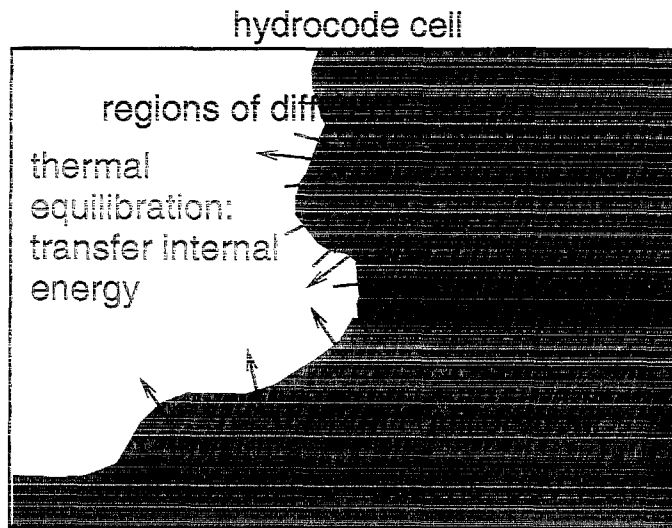
- Equation of state + constitutive model for each component (spatial region).

- Equilibration process for temperature and pressure.

- Strain enhancement around pores ⇒ extra plastic heating.

- Chemical reactions transfer mass between components.

- Regions may include multiple reacting chemicals.

Condensed-phase equations of state

- Need accurate temperature $\Rightarrow$ thermodynamically complete.

- Want to use QM EOS or harmonic model.

- Stop-gap: mechanical EOS + reference curve + heat capacity.

- Cold curve deduced from mechanical EOS fitted to shock data, with $\Gamma(\rho)$ model for off-Hugoniot states.

- Assumed constant c_v.

Constitutive model

For bulk of each component (where available):

- State: EOS (ρ, e) + elastic strain deviator + scalar plastic strain.

- Elastic $-$ plastic model used here.

Hotspot surface burn

Subcell model:

Reaction products occupy regions of a single characteristic size.

Shells of explosive reacting at products' temperature

reaction products

Bulk explosive reacts at bulk temperature and density.

Temperature and pressure equilibrated according to finite relaxation rates.

Surface burns with a flame speed, function of density and temperature.
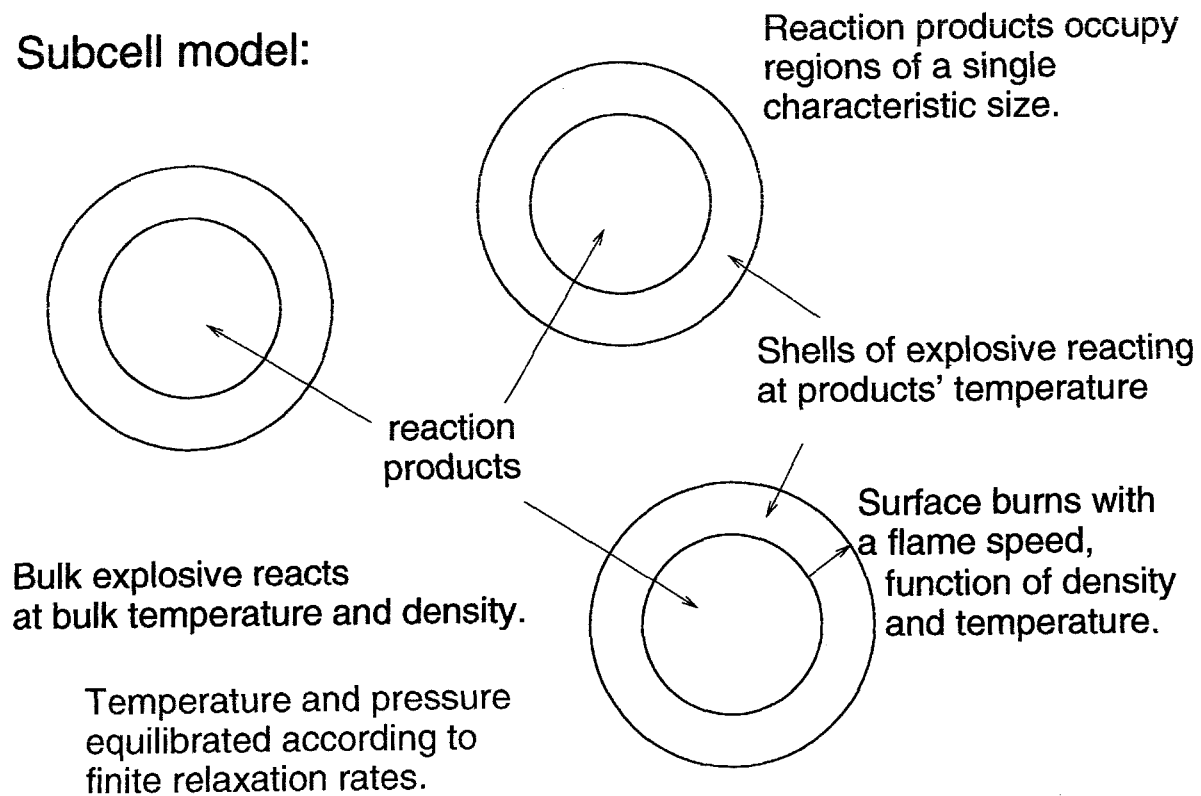
Enhanced plastic strain around pores

Subcell model:

More deformation => hotter.
(Weight to use in bulk reaction rate.)

Pores of a single
characteristic size

Bulk explosive deforms
with bulk velocity gradient.

Material near pores
deforms at higher rate,
depending on compression.
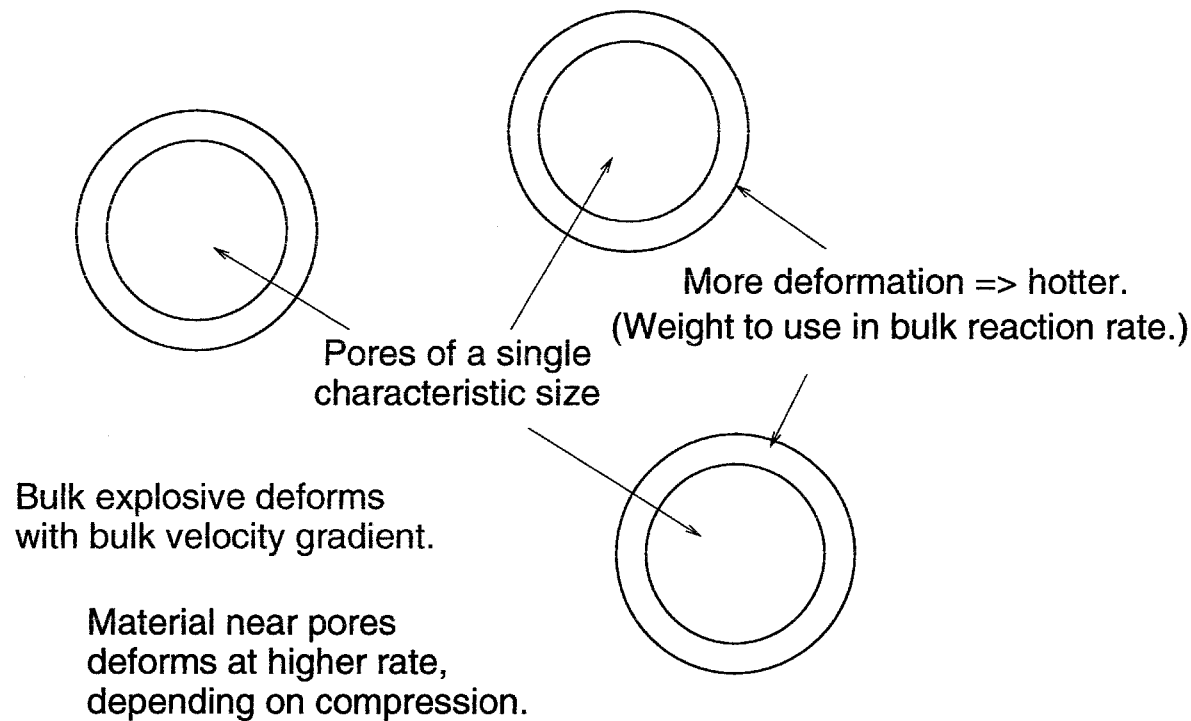
Velocity gradient (tensor) applied to bulk (component): $\mathrm{grad}\,\vec{u}$.

Internal pore $\Rightarrow$ variation in $\mathrm{grad}\,\vec{u}(\vec{r})$.

Consider $\mathrm{grad}\,\vec{u}$ at wall or pore:

$$\mathrm{grad}\,\vec{u}_{\mathsf{wall}} = \chi(\rho/\rho_0)\,M\,\mathrm{grad}\,\vec{u}_{\mathsf{bulk}}$$

where M is 3×3 strain mapping matrix, χ is compression function.

Choose M, χ to represent different microstructures.

Calibration (general)

– pure-component properties + microstructure.

- Pressure equilibration time: 'a few' times sound transit time for a grain.

- Temperature equilibration time: $\sim$order of magnitude larger.

- Surface burn area: common area between components i and j

$$a_{ij} \propto f_i^{2/3} f_j^{2/3},$$

  normalised to

$$a(1/2, 1/2) = 4\pi r^2 n$$

  where r is grain diameter, n is grain number density.

- Enhanced plastic flow: estimated from constant volume compression of hollow shell,

$$\chi(\rho/\rho_0) = \left[1 - \frac{\rho}{\rho_0}(1 - \nu_0)\right]^{-1/3}$$

  where ν_0 is initial porosity.

Explosive compositions

| explosive	components by mass	porosity
PBX 9404	HMX, 94%; NC, 3%; CEF, 3%	1.6%
PBX 9501	HMX, 95%; estane, 2.5%; BDNPA, 2.5%	1.6%
EDC37	HMX, 91%; K10, 8%; NC, 1%	0.18%

- Start with PBX 9501: maximum HMX, non-energetic binder.

- PBX 9404: energetic and stiffer binder.

- EDC37: energetic but liquid binder, low porosity.

Calibration (components)

- HMX EOS: Steinberg-type Grüneisen fit to shock data, Gibbs & Popolato heat capacity + expansivity.

- Polyurethane EOS: Steinberg-type Grüneisen fit to shock data, Lange heat capacity. (Slow-reacting binders treated as polyurethane.)

- NC EOS: assumed $u_s - u_p$ for cellulose acetate (Grüneisen fit), took $\rho_0 = 1.65\,\text{g/cm}^3$, estimated c_v.

- Products: temperature-dependent JWL for PBX 9404 – not sensitive for initiation.

- HMX reaction rate: calorimetry values from Gibbs & Popolato, adjusted to match PBX 9501 Pop plot.

- NC reaction rate: calorimetry values from Gibbs & Popolato.

- Slow-reacting binder rate: token value (not sensitive).

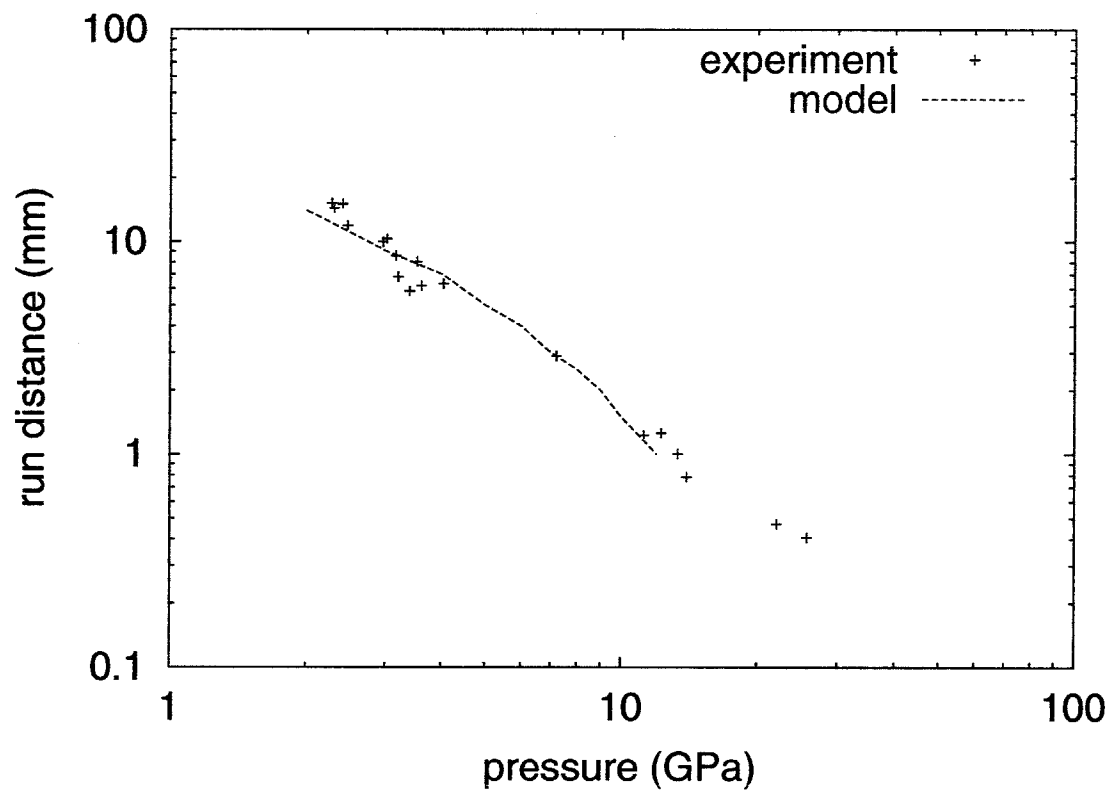- Initial porosity: nonzero volume fraction of products, STP state.

PBX 9501

Estimate $\tau_p = 0.1\,\mu s$, $\tau_T = 1.0\,\mu s$, $M_{12} = M_{13} = 1$;
fit to run distance data $T^* = 27000\,K$, $R_0 = 2 \times 10^7\,/\mu s$:
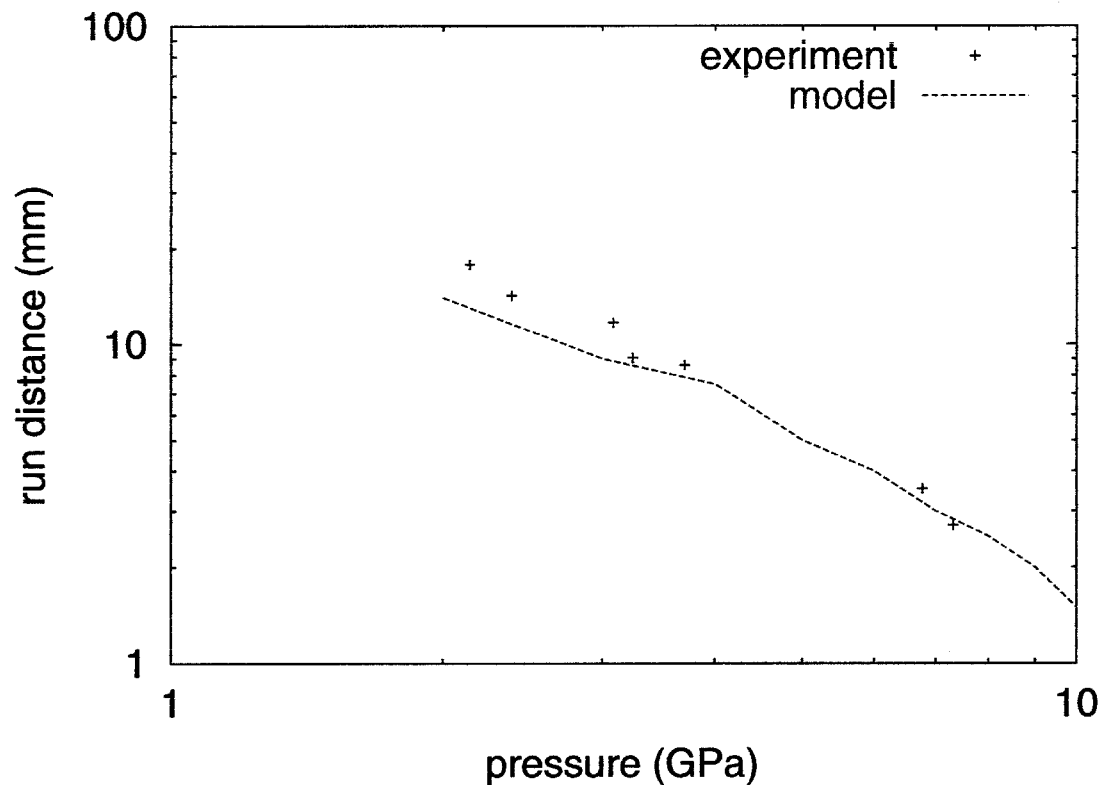
c.f. calorimetry value: 26500 K;
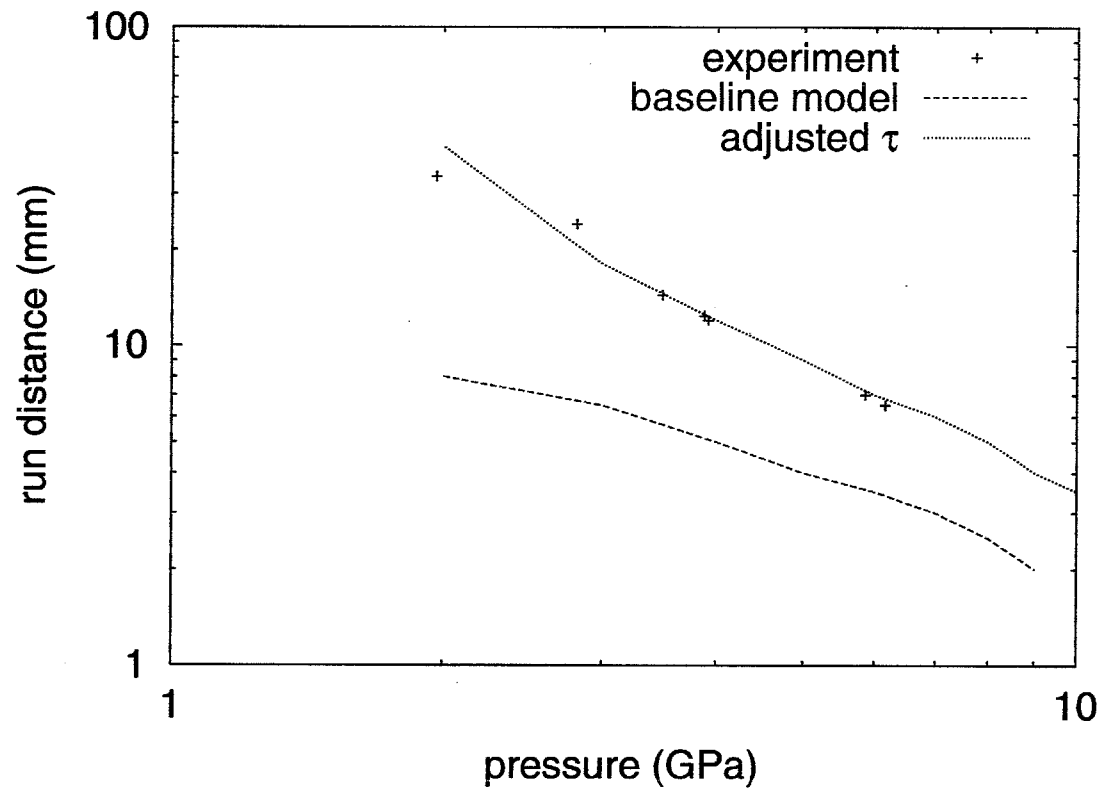R_0 consistent with atomic vibrations.

PBX 9404

Parameters as for PBX 9501,
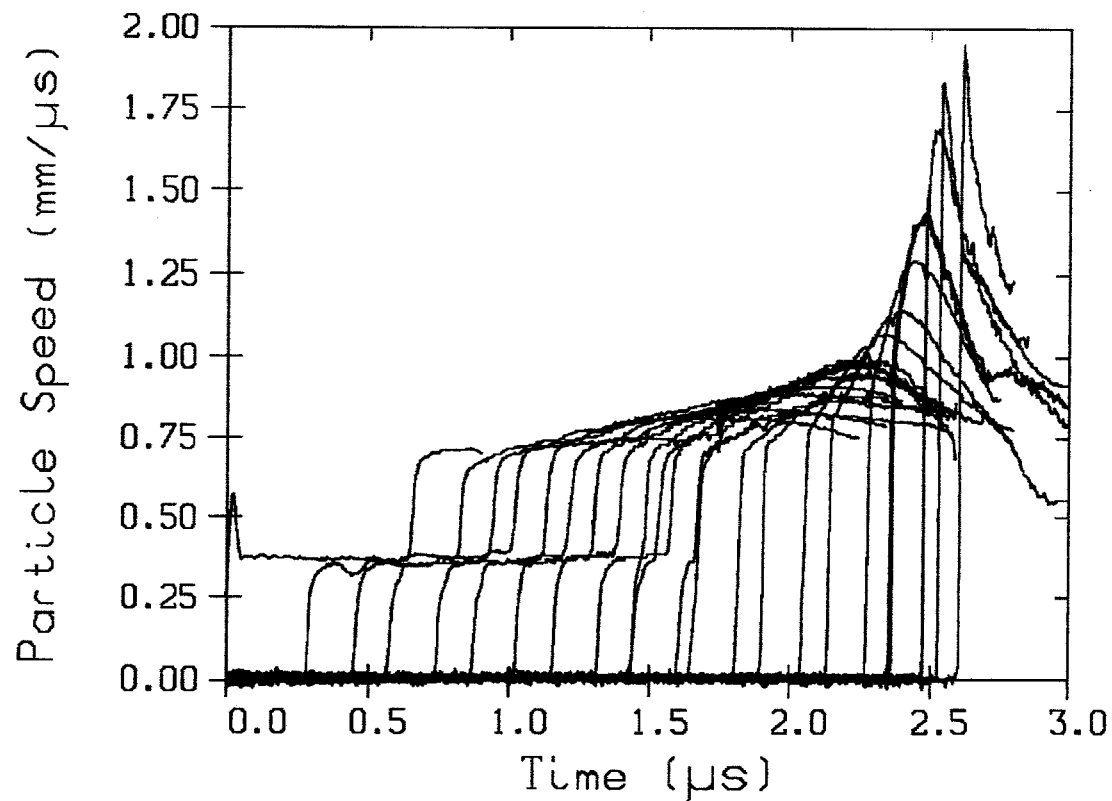except $M_{12} = M_{13} = 2$ (stiffer binder):

EDC37

Baseline: as for PBX 9501 except $M_{12} = M_{13} = 0$.

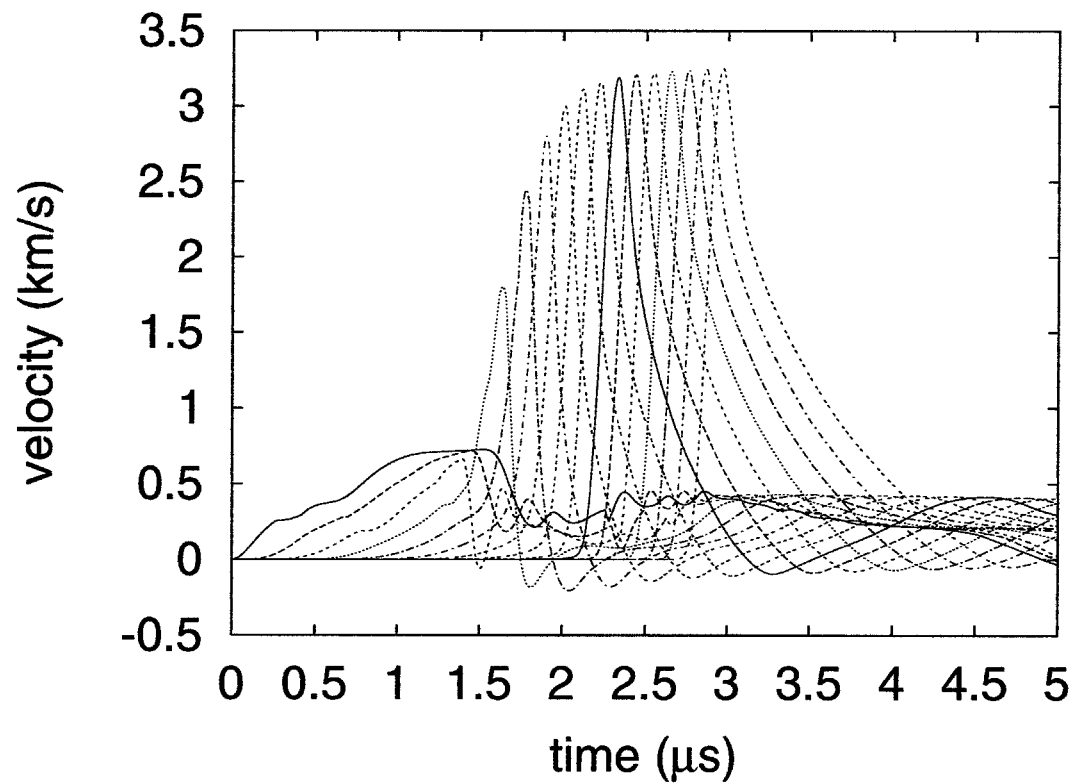Adjusted: $\tau_p = 0.013\,\mu\text{s}$, $\tau_T = 0.1\,\mu\text{s}$.

PBX 9404: particle velocity

Electromagnetic velocity gauge records from gas gun impact experiment:
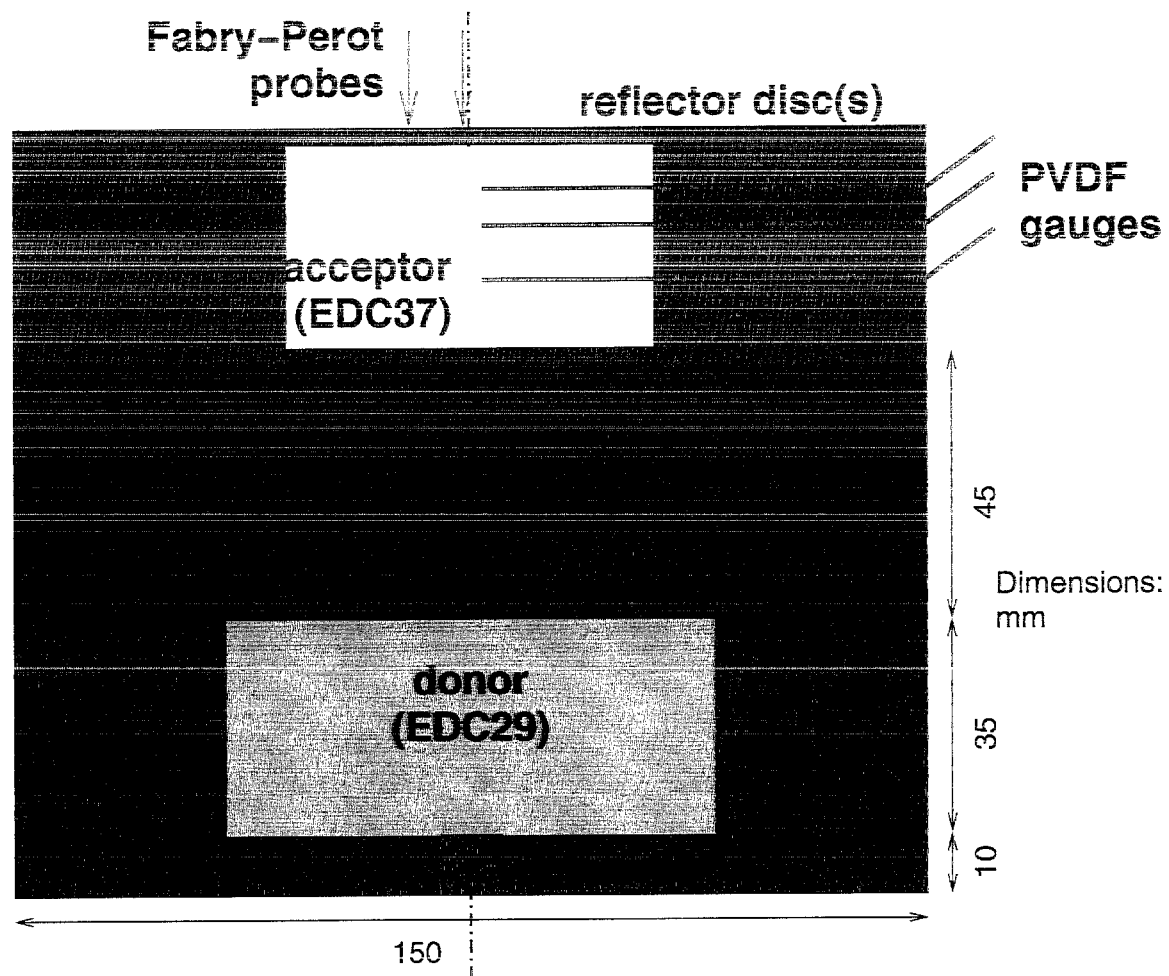
PBX 9404: particle velocity

Hydrocode simulation:

SI2D experiments

Fabry–Perot probes

reflector disc(s)

PVDF gauges

acceptor (EDC37)

donor (EDC29)

Dimensions: mm

45

35

10

150

EDC37: SI2D data
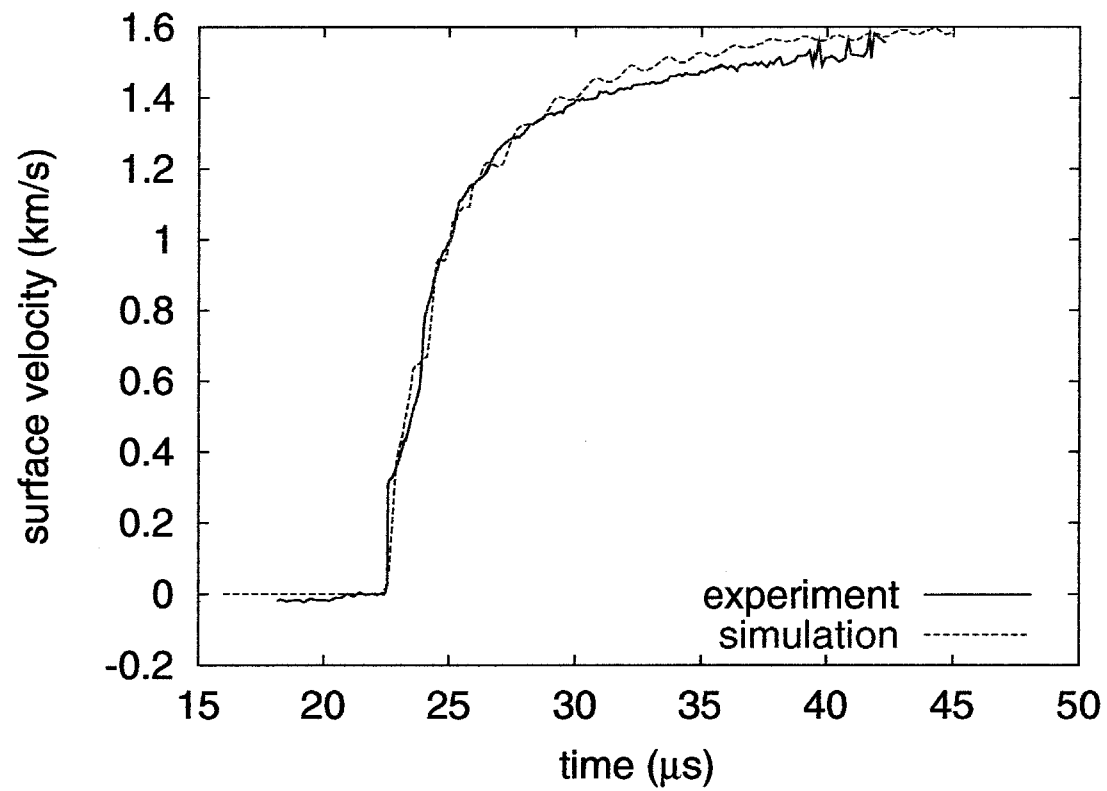
Summary and Conclusions

- Physically-based reactive flow model for HMX-based explosives.

- 'Coarse mesoscale' model of microstructure: physical constituents $+$ heterogeneous effects.

- Heterogeneous effects: equilibration, surface burn, plastic enhancement.

- Model can predict effect of composition, porosity.

- Trials so far: reasonable for run distance, velocity history and non-ideal performance.

- Models work quite well; some refinements desirable.

MESOSCALE MODELLING OF REACTION IN HMX-BASED EXPLOSIVES

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We are developing reactive flow models intended to have a wide
predictive capability covering composition and morphology,
in terms of composition, microstructure, and loading history,
while being reasonably efficient for design simulations.
We have concentrated on HMX-based formulations because of their
wide use as military explosives, and here we apply the model to
EDC37, which contains three energetic components.
Mesoscale models offer the most likely route, because it is important
to represent many cooperative and competing processes with adequate
accuracy.
Temperature-dependent reactions, based on
an Arrhenius decomposition rate in the bulk explosive, could
be used to reproduce aspects of the shock desensitisation observed
in HMX-based explosives [Mulford99a,Mulford99b].

For continuum mechanics simulations, explosive material was
represented as a heterogeneous mixture of components.
Each component was represented by its volume fraction,
a thermodynamically complete equation of state (EOS),
and a constitutive model if possible.
(In the models used previously, the only components considered were
'unreacted explosive' and 'reaction products' with no distinction
between explosive and binders.)
The mixture was allowed to equilibrate in pressure and temperature,
with an exponential relaxation rate towards the mean value.
Pressure equilibration was assumed to be isentropic.

Local Arrhenius reaction rates were used,
as this form is the most appropriate for chemical processes.
An additional hotspot term was included, whereby material at the surface
of reactive components was burnt at the temperature of the adjacent component.

The increased plastic flow around internal pores was modelled by
simulating the evolution of the state of the component adjacent to the
pore, as well as its bulk state.
This approach can be used to simulate hotspots originating from shear bands or
brittle failure rather than bulk plastic work, by modifying the form of the
equation or the values of its parameters.

EOS and constitutive models were used for each component of the
microstructure rather than for the complete mixture.
Thermodynamically complete EOS were estimated for each material.

The time constant for pressure equilibration was chosen by estimating
the characteristic time for sound to pass a few times across a
'typical' grain in the microstructure.
The time constant for thermal equilibrium
was estimated to be about an order of magnitude larger.
The density of common area between components was estimated
from the microstructure.
The model of plasticity enhancement around a pore was calibrated against

a simplified treatment of constant volume compression of a hollow shell.

Initial estimates of the Arrhenius parameters were taken from calorimetry
data [Gibbs80], and adjusted to reproduce initiation data.
The parameters for HMX were adjusted by considering PBX-9501 data,
as this composition does not have a reactive binder.

Porous materials were represented as before by starting with a non-zero
volume fraction of the reaction products at the STP state.

Parameters were deduced for PBX-9501, PBX-9404 and EDC37, all based on
HMX, but with different binders and porosities.
It was possible to reproduce Pop plots [Gibbs80] quite accurately using
an Arrhenius barrier close to the value for HMX deduced from calorimetry
data, and with a frequency factor close to the frequency for atomic
vibrations.
Variations in porosity were modelled by altering the equilibration times
for pressure and temperature.

Comparisons were made against velocity histories measured during
initiation by a single or double shock.
The new reactive flow model was able to reproduce the Pop plot and
desensitisation with reasonable accuracy.
Simulations were also made of experiments in which the drive produced by
an explosive was measured without allowing a fully-developed detonation
to form.

Mulford99a: R N Mulford and D C Swift, Reactive flow models
     for the desensitisation of high explosives,
     Proc International Workshop on Non-Ideal Explosives,
     held Socorro, New Mexico, USA, Mar 1999, EMRTC (2000).
Mulford99b: R N Mulford and D C Swift, Reactive flow models
     for the desensitisation of high explosives,
     Proc APS SCCM 1999, AIP (2000).
Gibbs80: T.R. Gibbs and A. Popolato, ``LASL Explosive Property Data''
     University of California Press, Berkeley (1980).
Gustavsen99: R.L. Gustavsen, S.A. Sheffield, R.R. Alcon,
     L.G. Hill, R.E. Winter, D.A. Salisbury and P. Taylor,
     Initiation of EDC37 measured with embedded electromagnetic
     particle velocity gauges,
     Proc APS SCCM 1999, AIP (1999).